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Some results on Laplacian spectral radius of graphs with cut vertices[☆]

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ABSTRACT

In this paper, we give some results on Laplacian spectral radius of graphs with cut vertices, and as their applications, we also determine the unique graph with the largest Laplacian spectral radius among all unicyclic graphs with n vertices and diameter d, $3 \leqslant d \leqslant n-3$.

1. Introduction

The graphs in this paper are simple and undirected. Let $G=(V,E)$ be a graph on vertex set $V(G)=\{v_1, v_2, \ldots, v_n\}$. For $v_i \in V(G)$, the *degree* of v_i, written $d_G(v_i)$ or $d(v_i)$, is the number of edges incident with v_i. The set of neighbors of a vertex v_i in G is denoted by $N_G(v_i)$, or briefly by $N(v_i)$. Its *adjacency matrix* is defined to be the $n \times n$ matrix $A(G)=(a_{ij})$, where $a_{ij}=1$ if v_i is adjacent to v_j, and $a_{ij}=0$ otherwise. Since $A(G)$ is a real symmetric matrix, its eigenvalues are all real. We call the largest eigenvalue of $A(G)$ the *spectral radius* of graph G, which is denoted by $\rho(G)$.

The *Laplacian matrix* is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees. The Laplacian characteristic polynomial of G is just $\det(xI - L(G))$, which is denoted by $\Phi(G,x)$, or simply by $\Phi(G)$. From the fact that $L(G)$ is a real symmetric matrix with row sums 0 and Geršgorin's theorem [14], it follows that its eigenvalues are nonnegative real numbers, and 0 is the smallest eigenvalue of $L(G)$. Hence the eigenvalues of $L(G)$ can be denoted by

$$\mu_1(G) \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_n(G) = 0,$$

in a non-increasing order. The largest eigenvalue $\mu_1(G)$ is the *Laplacian spectral radius* of graph G.

A *unicyclic* graph is a connected graph in which the number of edges equals the number of vertices. The *diameter* of a graph is the maximum distance between any pair of vertices. Let $\Diamond_n^d (3 \leqslant d \leqslant n-3)$ be a graph obtained from $C_4 = v_1v_2v_3v_4v_1$ by attaching $n-d-2$ pendent vertices together with a path of length $\left\lceil \frac{d}{2} \right\rceil - 1$ to vertex v_1, and a path of length $\left\lfloor \frac{d}{2} \right\rfloor - 1$ to vertex v_3. For example, see Fig. 6, if $k = \left\lceil \frac{d}{2} \right\rceil$, $G_1 \cong \Diamond_n^d$.

The investigation on the Laplacian spectral radius of graphs is an important topic in the theory of graph spectra. In the past few years, Guo [12] investigated how the Laplacian spectral radius changes when one graph is transferred to another graph obtained from the original graph by adding some edges, or subdivision, or removing some edges from one vertex to another; Guo [11] investigated how the Laplacian spectral radius behaves when the graph is perturbed by adding or grafting

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edges. At the same time, the problem concerning graphs with the maximal (minimal, respectively) Laplacian spectral radius of a given class of graphs has been studied extensively; see [4,10,19,20].

In this paper, we investigate the same problem on the graphs with cut vertices as above, and as their applications, we also obtain that $\lozenge_n^d$ is a unique graph with the largest Laplacian spectral radius among all unicyclic graphs with n vertices and fixed diameter d, for $3 \leqslant d \leqslant n-3$.

2. Some preliminaries

In this section, we will list some lemmas which will be used in Sections 3 and 4.

Let G be a graph. Let $G' := G + e$ be the graph obtained from G by inserting a new edge e into G. The well-known Courant–Weyl inequalities (see, e.g., [2], Theorem 2.1) imply the following interlacing theorem.

Lemma 2.1. $\mu_1(G') \geqslant \mu_1(G) \geqslant \mu_2(G') \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_n(G') = \mu_n(G) = 0$.

If $h(x)$ is a polynomial in variable x, let $\mu_1(h)$ denote the largest real root of equation $h(x) = 0$.

Lemma 2.2 (*[20]*)**.** *Let $h(x)$ and $g(x)$ be monic polynomials with real roots. If $h(x) < g(x)$ for all $x \geqslant \mu_1(g)$, then $\mu_1(h) > \mu_1(g)$.*

Remark. The above lemma remains valid if we replace $x \geqslant \mu_1(g)$ by $x \geqslant \mu_1(h)$.

Lemma 2.3 (*[2]*)**.** *Let A be a Hermitian matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ and B be one of its principal submatrices. Let B have eigenvalues $\mu_1, \ldots, \mu_m$. Then the inequalities $\lambda_{n-m+i} \leqslant \mu_i \leqslant \lambda_i (i = 1, \ldots, m)$ hold.*

Lemma 2.4 (*[5]*)**.** *Let A be a symmetric $n \times n$ matrix with eigenvalues $\theta_1 \geqslant \theta_2 \geqslant \cdots \geqslant \theta_n$. Then*

$$\theta_k = \max_{\dim(U)=k} \min_{x \in U} \frac{(x, Ax)}{(x, x)}$$

and the k-dimensional subspace for which the maximum occurs is unique, and is spanned by the eigenvectors associated with $\theta_1, \ldots, \theta_n$, where $\dim(U)$ denotes the dimension of the subspace U.

Lemma 2.5. *Let $G = (V_1, V_2; E)$ be a connected bipartite graph on n vertices and suppose that $V_1 = \{v_1, v_2, \ldots, v_j\}$, $V_2 = \{v_{j+1}, v_{j+2}, \ldots, v_n\}$. Let $X = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^t$ be a unit eigenvector of G corresponding to $\mu_1(G)$. Then we have*

(1) [7] *$B(G) = D(G) + A(G)$ and $L(G) = D(G) - A(G)$ are unitarily similar and the largest eigenvalue $\mu_1(G)$ of $L(G)$ is simple.*
(2) [11] $\mathrm{sgn}(x_{v_1}) = \cdots = \mathrm{sgn}(x_{v_j}) = -\mathrm{sgn}(x_{v_{j+1}}) = \cdots = -\mathrm{sgn}(x_{v_n}) \neq 0$.

Let $v_1, v_2, \ldots, v_n$ be a series of orthonormal eigenvectors corresponding to the eigenvalues $\mu_1(G + e), \mu_2(G + e), \ldots, \mu_n(G + e)$, respectively. Then we have

Lemma 2.6 (*[3]*)**.** *Let G be a simple graph of order n, $e = \{v_i, v_j\}$ $(i \neq j)$. If $\mu_r(G) = \mu_r(G+e) = \mu_r$, $r = 1, 2, \ldots, p$, $p \leqslant n-1$, then for each r $(r = 1, 2, \ldots, p)$, G and $G + e$ have the same orthonormal eigenvector v_r corresponding to μ_r for which the ith and jth entries are equal.*

The *Laplacian spectrum* of G is defined by the multiset $S(G) = \{\mu_1(G), \ldots, \mu_n(G)\}$. We say that the *Laplacian spectral variation* of G by adding an edge or a loop e is integral if the differences between the elements of $S(G + e) \setminus S(G)$ and $S(G) \setminus S(G + e)$ in the same places are integral.

Lemma 2.7 (*[17]*)**.** *Let G be a graph with nonadjacent vertices v_1 and v_2, and $\hat{G} = G + v_1v_2$. Then the Laplacian spectral integral variation occurs in one place if and only if vertices v_1 and v_2 have the same neighborhood in G. If the Laplacian spectral integral variation occurs in one place, the eigenvalue of G that increased by 2 is given by $d_G(v_1)$ (equivalently, $d_G(v_2)$).*

Lemma 2.8 (*[6,15]*)**.** *Let G be a connected graph on n vertices with at least one edge. Then $\mu_1(G) \geqslant \Delta(G) + 1$, where $\Delta(G)$ is the maximum degree of the graph G, with equality if and only if $\Delta(G) = n - 1$.*

Let G be a connected graph with $uv \in E(G)$. The graph $G_{u,v}$ is obtained from G by subdividing the edge uv, i.e., adding a new vertex w and edges wu, wv in $G - uv$. Hoffman and Smith define an *internal path* of G as a walk $v_0v_1 \cdots v_s (s \geqslant 1)$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $d(v_0) > 2$, $d(v_s) > 2$, and $d(v_i) = 2$, whenever $0 < i < s$. And s is called the length of the internal path. An internal path is closed if $v_0 = v_s$. They proved the following result.

Lemma 2.9 (*[13]*)**.** *Let uv be an edge of the connected graph G on n vertices.*

(i) *If uv does not belong to an internal path of G, and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$.*
(ii) *If uv belongs to an internal path of G, and $G \neq W_n$, where W_n is shown in Fig. 1, then $\rho(G_{u,v}) < \rho(G)$.*

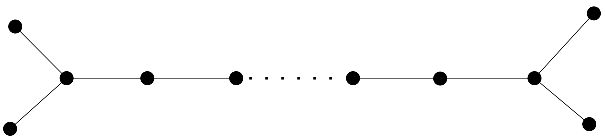

Fig. 1. W_n.

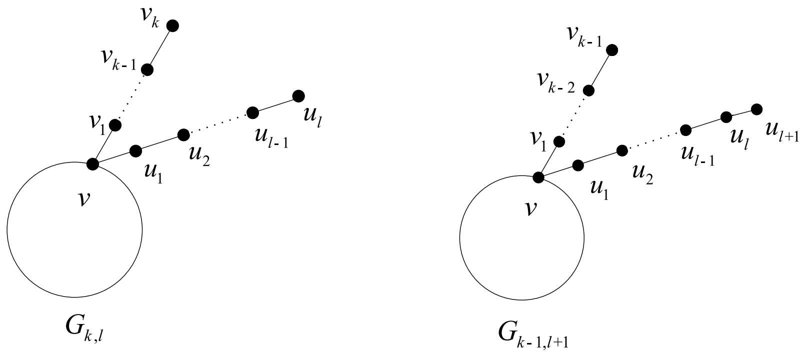

Fig. 2. Graphs $G_{k,l}$ and $G_{k-1,l+1}$.

In the following, we denote by $G^{uv}(w)$ the graph obtained from G by contracting edge $e = uv$, where e is an arbitrary edge of G and w is the new vertex.

Lemma 2.10 ([18]). *Let $e = uv$ be an arbitrary edge of a tree $T = (V, E)$. Then*

(1) *If uv does not belong to an interval path, then $\mu_1(T^{uv}(w)) < \mu_1(T)$.*
(2) *If uv belongs to an interval path, then $\mu_1(T^{uv}(w)) > \mu_1(T)$.*

Here, we generalize the above lemma to bipartite graphs. Since their proofs are almost the same, here we omit it.

Corollary 2.11. *Let $e = uv$ be an arbitrary edge of a bipartite graph $G = (V, E)$. Then*

(1) *If uv does not belong to an interval path, then $\mu_1(G^{uv}(w)) < \mu_1(G)$.*
(2) *If uv belongs to an interval path and $G^{uv}(w)$ is still a bipartite graph, then $\mu_1(G^{uv}(w)) > \mu_1(G)$.*

Lemma 2.12 ([11]). *Let u, v be two vertices of a connected bipartite graph $G = (V_1, V_2, E)$. Suppose that $v_1, v_2, \ldots, v_s (1 \leqslant s \leqslant d(v))$ are some vertices of $N_G(v) \setminus N_G(u)$ different from u. Let X be a unit eigenvector of G corresponding to $\mu_1(G)$, and let G^* be the graph obtained from G by deleting the edges vv_i and adding the edges $uv_i (1 \leqslant i \leqslant s)$. If $|x_u| \geqslant |x_v|$ and G^* is also a bipartite graph, then $\mu_1(G^*) > \mu_1(G)$.*

The *line graph* L^G of a graph G is constructed by taking the edges of G as vertices of L^G, and joining two vertices in L^G by an edge whenever the corresponding edges in G have a common vertex.

Lemma 2.13 ([16]). *$\mu_1(G) \leqslant 2 + \rho(L^G)$, the equality holds if and only if G is a bipartite graph.*

Lemma 2.14 ([9]). *Let G be a connected bipartite graph and H a subgraph of G. Then $\mu_1(H) \leqslant \mu_1(G)$, and the equality holds if and only if $G = H$.*

Lemma 2.15 ([8]). *Let G be a unicyclic graph of order n. Then $\mu_1(G) \geqslant \mu_1(C_n)$ and the equality holds if and only if $G \cong C_n$.*

Lemma 2.16 ([11]). *Let G be a connected graph on n vertices and v be a vertex of G. Let $G_{k,l}$ be the graph defined as in Fig. 2. If $l \geqslant k \geqslant 1$, then*

$$\mu_1(G_{k-1,l+1}) \leqslant \mu_1(G_{k,l}),$$

with equality if and only if there exists a unit eigenvector of $G_{k,l}$ corresponding to $\mu_1(G_{k,l})$ taking the value 0 on vertex v. Especially, the inequality is strict if G is a bipartite graph.

3. Some results about graphs with cut vertices

Let $Gu : vH$ denote the graph formed by only identifying the vertex u of G with the vertex v of H (see Fig. 3). If u and v are two vertices of G, let $L_{u,v}(G)$ denote the principal submatrix of $L(G)$ formed by deleting the rows and the columns

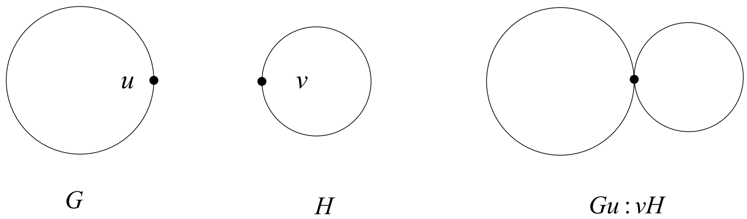

Fig. 3. Graph $Gu : vH$.

corresponding to vertices u and v. Then $L_u(G)$ can be defined similarly. In the following, we always use $\Phi(L_u(G))$ and $\Phi(L_{u,v}(G))$ to denote the characteristic polynomials of $L_u(G)$ and $L_{u,v}(G)$, respectively.

Enlightened by the formula about the characteristic polynomial of graphs formed by pasting two graphs together (see [1], Theorem 9.1), we get the following lemma:

Lemma 3.1. *Let $G = G_1u : vG_2$. Then*

$$\Phi(G) = \Phi(G_1)\Phi(L_v(G_2)) + \Phi(L_u(G_1))\Phi(G_2) - x\Phi(L_u(G_1))\Phi(L_v(G_2)). \tag{3.1}$$

Proof. Suppose $V(G_1) = \{u_1, \dots, u_{n-1}, u\}$ and $V(G_2) = \{v, v_2, \dots, v_m\}$. We may assume that u and v are identified as a new single vertex u^*. The rows of the Laplacian matrix of G can be ordered by $u_1, \dots, u_{n-1}, u^*, v_2, \dots, v_m$. Let $L(G_1) = (l_{ij})_{n\times n}$, $L(G_1) = (r_{ij})_{m\times m}$, $l = (l_{n1}, \dots, l_{n-1,1})^t$, $r = (l_{12}, \dots, l_{1m})^t$, $O = (0)_{(n-1)\times(m-1)}$, $O_1 = (0)_{(m-1)\times 1}$, $O_2 = (0)_{(n-1)\times 1}$. Then

$$\begin{aligned}
\Phi(L(G)) &= \begin{vmatrix} xI_{n-1} - L_u(G_1) & -l & O \\ -l^t & x - d_{G_1}(u) - d_{G_2}(v) & -r^t \\ O^t & -r & xI_{m-1} - L_v(G_2) \end{vmatrix} \\
&= \begin{vmatrix} xI_{n-1} - L_u(G_1) & -l & O \\ -l^t & x - d_{G_1}(u) & -r^t \\ O^t & O_1 & xI_{m-1} - L_v(G_2) \end{vmatrix} + \begin{vmatrix} xI_{n-1} - L_u(G_1) & O_2 & O \\ -l^t & x - d_{G_2}(v) & -r^t \\ O^t & -r & xI_{m-1} \end{vmatrix} \\
&\quad + \begin{vmatrix} xI_{n-1} - L_u(G_1) & O_2 & O \\ -l^t & -x & -r^t \\ O^t & O_1 & xI_{m-1} - L_v(G_2) \end{vmatrix} \\
&= \Phi(G_1)\Phi(L_v(G_2)) + \Phi(L_u(G_1))\Phi(G_2) - x\Phi(L_u(G_1))\Phi(L_v(G_2)). \quad \square
\end{aligned}$$

Lemma 3.2. *For all $x \geqslant \mu_1(G)$, we have*

$$\Phi(G) - x\Phi(L_u(G)) \leqslant 0,$$

the equality holds if and only if $x = \mu_1(G) = \mu_1(L_u(G))$.

Proof. Let $|V(G)| = n$. Since $L_u(G)$ is the principal submatrix of $L(G)$ formed by deleting the row and the column corresponding to vertex u, by Lemma 2.3, we have

$$\mu_{i+1}(G) \leqslant \mu_i(L_u(G)) \leqslant \mu_i(G) \quad (i = 1, \dots, n-1),$$

i.e.,

$$\mu_1(G) \geqslant \mu_1(L_u(G)) \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_{n-1}(G) \geqslant \mu_{n-1}(L_u(G)) \geqslant \mu_n(G) = 0.$$

So

$$\Phi(G) - x\Phi(L_u(G)) = x\left[\prod_{i=1}^{n-1}(x - \mu_i(G)) - \prod_{i=1}^{n-1}(x - \mu_i(L_u(G)))\right].$$

If $x > \mu_1(G)$, we have

$$0 < x - \mu_i(G) \leqslant x - \mu_i(L_u(G)) \quad (i = 1, \dots, n-1).$$

Since

$$\sum_{i=1}^{n-1}\mu_i(G) = \sum_{i=1}^{n}\mu_i(G) = \mathrm{tr}(L(G)) > \mathrm{tr}(L_u(G)) = \sum_{i=1}^{n-1}\mu_i(L_u(G)),$$

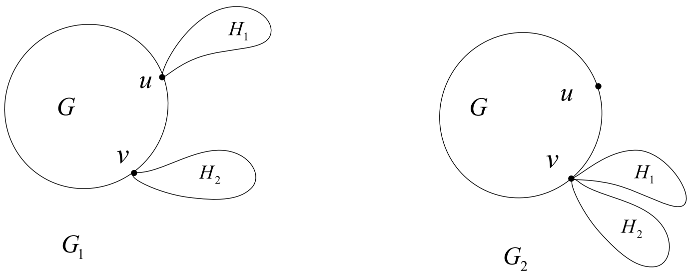

Fig. 4. Graphs G_1 and G_2.

there must exist some $1 \leqslant k \leqslant n-1$ such that $x - \mu_i(G) < x - \mu_i(L_u(G))$. So, in this case, we have

$$\Phi(G) - x\Phi(L_u(G)) < 0.$$

If $x = \mu_1(G)$, we have

$$\Phi(G) - x\Phi(L_u(G)) = 0 - \mu_1(G)\prod_{i=1}^{n-1}(\mu_1(G) - \mu_i(L_u(G))) \leqslant 0,$$

and the equality holds if and only if $\mu_1(G) = \mu_1(L_u(G))$.

This completes the proof. $\square$

Lemma 3.3. *Let $X = (x_1, x_2, \ldots, x_n)^t$ be a unit eigenvector of G corresponding to $\mu_1(G)$, where x_i corresponds to the vertex $u_i (1 \leqslant i \leqslant n)$. If $\mu_1(G)$ is simple, then for some $1 \leqslant k \leqslant n$, $\mu_1(G) = \mu_1(L_{u_k}(G))$ if and only if $x_k = 0$.*

Proof. For the necessity, we may assume that $L_{u_k}(G)Y = \mu_1(L_{u_k}(G))Y$, where $Y = (y_1, y_2, \ldots, y_{k-1}, y_{k+1}, \ldots, y_n)^t$ is a unit eigenvector of $L_{u_k}(G)$ corresponding to $\mu_1(L_{u_k}(G))$. Let $X' = (y_1, y_2, \ldots, y_{k-1}, 0, y_{k+1}, \ldots, y_n)^t$. Then $\mu_1(G) = \frac{(X', L(G)X')}{(X', X')} = \frac{(Y, L_{u_k}(G)Y)}{(Y,Y)} = \mu_1(L_{u_k}(G))$.

Since $\mu_1(G) = \max_{\dim(U)=1}\min_{X^* \in U}\frac{(X^*, AX^*)}{(X^*, X^*)}$, by Lemma 2.4, we get that X' is a unit eigenvector of G corresponding to $\mu_1(G)$, and the 1-dimensional subspace for which the maximum occurs is spanned by X'. Since $\mu_1(G)$ is simple, we get $X = bX'$, where b is a nonzero constant. So $x_k = 0$.

For the sufficiency, let $Y = (x_1, x_2, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n)^t$. Then $L_{u_k}(G)Y = \mu_1(G)Y$, by Lemma 2.4, $\mu_1(L_{u_k}(G)) \geqslant \frac{(Y, L_{u_k}(G)Y)}{(Y,Y)} = \mu_1(G)$. By Lemma 2.3, we get $\mu_1(L_{u_k}(G)) \leqslant \mu_1(G)$. So $\mu_1(G) = \mu_1(L_{u_k}(G))$. $\square$

Lemma 3.4. *Let G_1 and G_2 be shown as in Fig. 4, $G_1 = H_1u^* : uGv : v^*H_2$ and $G_2 = H_1u^* : vGv : v^*H_2$. If $\Phi(L_u(G)) \leqslant \Phi(L_v(G))$ for all $x \geqslant \mu_1(G_1)$, then $\mu_1(G_1) \leqslant \mu_1(G_2)$. In particular, the inequality is strict if H_1 and H_2 are both bipartite graphs.*

Proof. By Lemma 3.1, we have

$$\begin{aligned}\Phi(G_1) &= \Phi(L_{u^*}(H_1))\Phi(Gv : v^*H_2) + \Phi(L_u(Gv : v^*H_2))(\Phi(H_1) - x\Phi(L_{u^*}(H_1)))\\ &= \Phi(L_{u^*}(H_1))\Phi(Gv : v^*H_2) + [\Phi(L_u(G))\Phi(L_{v^*}(H_2))\\ &\quad + \Phi(L_{u,v}(G))(\Phi(H_2) - x\Phi(L_{v^*}(H_2)))](\Phi(H_1) - x\Phi(L_{u^*}(H_1)));\end{aligned}$$

$$\Phi(G_2) = \Phi(L_{u^*}(H_1))\Phi(Gv : v^*H_2) + \Phi(L_v(G))\Phi(L_{v^*}(H_2))(\Phi(H_1) - x\Phi(L_{u^*}(H_1)))$$

$$\begin{aligned}\Phi(G_1) - \Phi(G_2) &= (\Phi(H_1) - x\Phi(L_{u^*}(H_1)))[(\Phi(L_u(G)) - \Phi(L_v(G)))\Phi(L_{v^*}(H_2))\\ &\quad + \Phi(L_{u,v}(G))(\Phi(H_2) - x\Phi(L_{v^*}(H_2)))].\end{aligned}$$

By Lemma 3.2, for all $x \geqslant \mu_1(G_1)$, $\Phi(H_1) - x\Phi(L_{u^*}(H_1)) \leqslant 0$; $\Phi(L_u(G)) - \Phi(L_v(G)) \leqslant 0$; $\Phi(H_2) - x\Phi(L_{v^*}(H_2)) \leqslant 0$. So $\Phi(G_1) - \Phi(G_2) \geqslant 0$, for all $x \geqslant \mu_1(G_1)$. By Lemma 2.2, $\mu_1(G_1) \leqslant \mu_1(G_2)$.

We assume that X, Y are two unit eigenvectors of H_1, H_2 corresponding to $\mu_1(H_1), \mu_1(H_2)$, respectively. If H_1 and H_2 are both bipartite graphs, by Lemma 2.5, $\mu_1(H_1)$ and $\mu_1(H_2)$ are both simple and $x_{u^*} \neq 0$, $y_{v^*} \neq 0$. By Lemma 3.3, $\mu_1(H_1) > \mu_1(L_{u^*}(H_1))$, $\mu_1(H_2) > \mu_1(L_{v^*}(H_2))$. By Lemma 3.2, for all $x \geqslant \mu_1(G_1)$, $\Phi(H_1) - x\Phi(L_{u^*}(H_1)) < 0$; $\Phi(H_2) - x\Phi(L_{v^*}(H_2)) < 0$. So $\Phi(G_1) - \Phi(G_2) > 0$, for all $x \geqslant \mu_1(G_1)$. By Lemma 2.2, we get $\mu_1(G_1) < \mu_1(G_2)$. $\square$

In the above lemma, we say that G_2 can be obtained from G_1 by carrying out a transformation.

Lemma 3.5. *Let G be a connected graph of order n and X a unit eigenvector of G corresponding to $\mu_1(G)$. If there exist three different vertices v_i, v_{i+1}, v_j such that $x_{v_i} \leqslant x_{v_{i+1}} \leqslant x_{v_j}$ and v_i is adjacent to v_{i+1}, v_j is nonadjacent to v_i. Then $\mu_1(G) \leqslant \mu_1(G - v_iv_{i+1} + v_iv_j)$. Especially, the inequality is strict if $x_{v_{i+1}} \neq x_{v_j}$.*

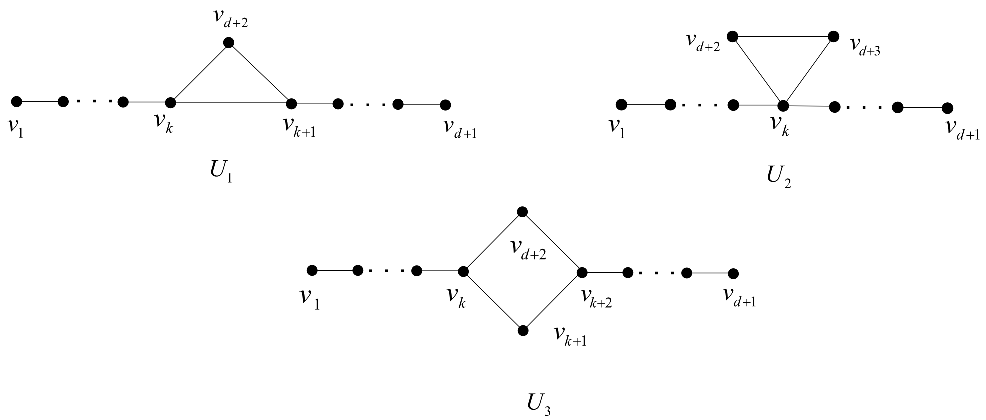

Fig. 5. Graphs U_1, U_2 and U_3.

Proof. Let $G' = G - v_iv_{i+1} + v_iv_j$. Then

$$\begin{aligned}\mu_1(G') - \mu_1(G) &\geqslant X^tL(G')X - X^tL(G)X\\ &= X^t(L(G') - L(G))X\\ &= x_{v_j}^2 - x_{v_{i+1}}^2 - 2x_{v_i}x_{v_j} + 2x_{v_i}x_{v_{i+1}}\\ &= (x_{v_j} - x_{v_{i+1}})(x_{v_j} + x_{v_{i+1}} - 2x_{v_i})\\ &\geqslant 0.\end{aligned}$$

So $\mu_1(G) \leqslant \mu_1(G - v_iv_{i+1} + v_iv_j)$ and the inequality is strict if $x_{v_{i+1}} \neq x_{v_j}$. $\square$

4. Applications

If the subgraph induced by the vertices of a path P in G is P itself, we call P an *induced path*. In the following, we use $\mathcal{U}_n^d$ to denote the sets of all unicyclic graphs with n vertices and diameter d. Let U_i $(i = 1, 2, 3)$ be three unicyclic graphs shown in Fig. 5. Let $U_i(p_2, \ldots, p_d, p_{d+2})$ $(i = 1, 3)$ and $U_2(p_2, \ldots, p_d, p_{d+2}, p_{d+3})$ be three classes of graphs of order n obtained from U_i $(i = 1, 2, 3)$ by attaching a tree T_j to each $v_j \in V(U_i) \setminus \{v_1, v_{d+1}\}$ $(i = 1, 2, 3)$, respectively, where $V(T_j)$ contains vertex v_j and $|V(T_j)| = p_j + 1$.

Let

$$\widetilde{\mathcal{U}}_i^d = \bigcup_{\Sigma_{j=2}^d p_j + p_{d+2} = n-d-2} U_i(p_2, \ldots, p_d, p_{d+2}), \quad i = 1, 3;$$

$$\widetilde{\mathcal{U}}_2^d = \bigcup_{\Sigma_{j=2}^d p_j + p_{d+2} + p_{d+3} = n-d-3} U_2(p_2, \ldots, p_d, p_{d+2}, p_{d+3});$$

$$\overline{\mathcal{U}}_3^d = \bigcup_{p_j = n-d-2} U_3(0, \ldots, 0, p_j, 0, \ldots, 0).$$

In the following, we denote by $G[S]$ the induced subgraph of G, for $S \subseteq V(G)$.

Lemma 4.1. *For any graph $G \in \widetilde{\mathcal{U}}_1^d$, there exists a graph $G^* \in \widetilde{\mathcal{U}}_3^d$ such that $\mu_1(G) < \mu_1(G^*)$.*

Proof. For any graph $G \in U_1(p_2, \ldots, p_d, p_{d+2}) \subseteq \widetilde{\mathcal{U}}_1^d$, let T_i be the tree attached to the vertex v_i of U_1, for $i = 2, \ldots, d, d+2$. Let $C = v_kv_{k+1}v_{d+2}v_k$ be the unique cycle of G. If $p_{d+2} > 0$, let $G_1 = G[V(T_2) \cup \cdots \cup V(T_k) \cup \{v_1, v_{k+1}, v_{d+2}\}]$, $G_2 = T_{d+2}$, $G_3 = G[V(T_{k+1}) \cup \cdots \cup V(T_d) \cup \{v_{d+1}\}]$. Then $G = G_2v_{p+2} : v_{p+2}G_1v_{k+1} : v_{k+1}G_3$ and G_2, G_3 are bipartite graphs. Let $G' = G_2v_{p+2} : v_{k+1}G_1v_{k+1} : v_{k+1}G_3$. Since $\Phi(L_{v_{p+2}}(G_1)) = \Phi(L_{v_{k+1}}(G_1))$ for all $x \geqslant \mu_1(G)$, by Lemma 3.4, we have $\mu_1(G) < \mu_1(G')$. From G to G', only the following distances are changed: the distances between the vertices of $V(G_2)\setminus\{v_{d+2}\}$ and v_{d+2} are increased by one, and the distances between the vertices of $V(G_2) \setminus \{v_{d+2}\}$ and the vertices of $V(G_3) \cup \{v_{k+1}\}$ are decreased by one. Then $G' \in \widetilde{\mathcal{U}}_1^d$. So in the following, we can consider G' instead of G, or we may assume that $p_{d+2} = 0$ directly. Similarly, we can assume that T_k and T_{k+1} are stars in G. This is because, we assume that T_{k+1} is not a star, then there must exist at least one edge $e = uv \in E(T_{k+1})$ such that each component of $G - e$ contains at least two vertices. Let $G_1 = e$ and denote the two components of $G - e$ by G_2, G_3, respectively. Then $G = G_2u : uG_1v : vG_3$. Let $G' = G_2u : vG_1v : vG_3$. Then $G' \in \widetilde{\mathcal{U}}_1^d$. Since $\Phi(L_u(G_1)) = \Phi(L_v(G_1))$ for all $x \geqslant \mu_1(G)$, by Lemma 3.4, we have $\mu_1(G) \leqslant \mu_1(G')$. Again we can consider G' instead of G, or we may assume that T_k and T_{k+1} are stars. So, for convenience, we assume that $p_{d+2} = 0$ and T_k, T_{k+1} are stars in G.

Case 1. $p_k p_{k+1} = 0$.

We may assume that $p_{k+1} = 0$. Let $G^* = G - v_{k+1}v_{d+2} + v_{k+2}v_{d+2}$ and $G' = G + v_{k+2}v_{d+2}$. Then $G^* \in U_3(p_2, \ldots, p_{k-1}, p_k, 0, p_{k+2}, \ldots, p_d, 0) \subseteq \widetilde{\mathcal{U}}_3^d$. Since $N_{G^*}(v_{d+2}) = N_{G^*}(v_{k+1})$, by Lemma 2.7, from G^* to G', the Laplacian spectral integral variation occurs in one place and the eigenvalue of G^* that increased by 2 is given by the degree of the vertex v_{d+2}. By Lemma 2.8, $\mu_1(G^*) > \Delta(G^*) + 1 > 4 \geqslant d_{G^*}(v_{d+2}) + 2$, this means, from G^* to G', $\mu_1(G^*)$ is unchanged, i.e., $\mu_1(G^*) = \mu_1(G')$. Since $G' = G + v_{k+2}v_{d+2}$, by Lemma 2.1, $\mu_1(G) \leqslant \mu_1(G')$. If $\mu_1(G) = \mu_1(G')$, let $X^{(1)}, X^{(2)}, \ldots, X^{(n)}$ be a series of orthonormal eigenvectors corresponding to the eigenvalues $\mu_1(G'), \mu_2(G'), \ldots, \mu_n(G')$, respectively. Then by Lemma 2.6, we get that G, G^*, G' have the same eigenvector $X^{(1)}$ corresponding to $\mu_1(G')$ of which the $(k+2)$th and the $(d+2)$th entries are equal. Since G^* is a bipartite graph, by Lemma 2.5, $\mathrm{sgn}(X^{(1)}_{v_{k+2}}) = -\mathrm{sgn}(X^{(1)}_{v_{d+2}}) \neq 0$, which is a contradiction. So $\mu_1(G) < \mu_1(G^*)$.

Case 2. $p_k p_{k+1} \neq 0$.

Suppose that $X = (x_1, \ldots, x_n)^t$ is a unit eigenvector of G corresponding to $\mu_1(G)$, where x_i corresponds to vertex $v_i (1 \leqslant i \leqslant n)$. Since $-X$ is also a unit eigenvector corresponding to $\mu_1(G)$, we may assume that $x_k + x_{k+1} \geqslant 0$ and $x_k \geqslant x_{k+1}$. Suppose that v_t is a pendent vertex attached to v_{k+1}. Now, we prove that $\mu_1(G) \leqslant \mu_1(G - v_{k+1}v_t + v_k v_t)$.

Since $L(G)X = \mu_1(G)X$, we get $\mu_1(G)x_i = d(v_i)x_i - \sum_{v_j \in N(v_i)} x_j$. So

$$x_t = \frac{-x_{k+1}}{\mu_1(G) - 1}, \qquad x_{d+2} = \frac{x_k + x_{k+1}}{2 - \mu_1(G)}.$$

If $x_{k+1} \geqslant 0$, let $G'' = G - v_{k+1}v_t + v_k v_t$. Then we have $x_t \leqslant 0$ and

$$\begin{aligned}\mu_1(G'') - \mu_1(G) &\geqslant X^t L(G'')X - X^t L(G)X \\ &= X^t(L(G'') - L(G))X \\ &= x_k^2 - x_{k+1}^2 + 2x_t x_{k+1} - 2x_t x_k \\ &= (x_k - x_{k+1})(x_k + x_{k+1} - 2x_t) \\ &\geqslant 0.\end{aligned}$$

If $x_{k+1} < 0$, let $G'' = G - v_{k+1}v_{d+2} + v_k v_t$. Then

$$\begin{aligned}\mu_1(G'') - \mu_1(G) &\geqslant X^t L(G'')X - X^t L(G)X \\ &= X^t(L(G'') - L(G))X \\ &= x_k^2 + x_t^2 - x_{d+2}^2 - x_{k+1}^2 + 2x_{k+1}x_{d+2} - 2x_k x_t \\ &= (x_k - x_t)^2 - (x_{k+1} - x_{d+2})^2 \\ &= \left(x_k + \frac{x_{k+1}}{\mu_1(G) - 1}\right)^2 - \left(\frac{x_k + x_{k+1}}{\mu_1(G) - 2} + x_{k+1}\right)^2 \\ &= \left(\frac{(\mu_1(G) - 1)x_k + x_{k+1}}{\mu_1(G) - 1}\right)^2 - \left(\frac{x_k + (\mu_1(G) - 1)x_{k+1}}{\mu_1(G) - 2}\right)^2,\end{aligned}$$

if $x_k + (\mu_1(G) - 1)x_{k+1} \geqslant 0$, then

$$\frac{(\mu_1(G) - 1)x_k + x_{k+1}}{\mu_1(G) - 1} + \frac{x_k + (\mu_1(G) - 1)x_{k+1}}{\mu_1(G) - 2} > 0,$$

$$\frac{(\mu_1(G) - 1)x_k + x_{k+1}}{\mu_1(G) - 1} - \frac{x_k + (\mu_1(G) - 1)x_{k+1}}{\mu_1(G) - 2} = \frac{(\mu_1(G) - 1)(\mu_1(G) - 3)x_k - (\mu_1(G)^2 - 3\mu_1(G) + 3)x_{k+1}}{(\mu_1(G) - 1)(\mu_1(G) - 2)} > 0;$$

if $x_k + (\mu_1(G) - 1)x_{k+1} < 0$, then

$$\frac{(\mu_1(G) - 1)x_k + x_{k+1}}{\mu_1(G) - 1} + \frac{x_k + (\mu_1(G) - 1)x_{k+1}}{\mu_1(G) - 2} > \frac{\mu_1(G)x_k + \mu_1(G)x_{k+1}}{\mu_1(G) - 1} \geqslant 0,$$

$$\frac{(\mu_1(G) - 1)x_k + x_{k+1}}{\mu_1(G) - 1} - \frac{x_k + (\mu_1(G) - 1)x_{k+1}}{\mu_1(G) - 2} > 0.$$

In either case, $\mu_1(G'') \geqslant \mu_1(G)$.

Since $G'' \cong G - v_{k+1}v_t + v_k v_t$, we get $\mu_1(G - v_{k+1}v_t + v_k v_t) \geqslant \mu_1(G)$.

Let X'' be a unit eigenvector of G'' corresponding to $\mu_1(G'')$ such that $x''_k + x''_{k+1} \geqslant 0$. Then $x''_k \geqslant x''_{k+1}$. Otherwise, $x''_k < x''_{k+1}$. Using a similar way to Case 2, we can get $\mu_1(G'') < \mu_1(G)$, which is a contradiction.

Repeat the above procedure until there is no pendent vertex attached to v_{k+1}. We denote the final graph by G''', then $\mu_1(G) \leqslant \mu_1(G''')$. For G''', since $p'''_{k+1} = 0$, according to Case 1, we can find a graph $G^* \in \widetilde{\mathcal{U}}_3^d$ such that $\mu_1(G''') < \mu_1(G^*)$. So $\mu_1(G) < \mu_1(G^*)$.

We complete the proof. $\square$

Lemma 4.2. *For any graph $G \in \widetilde{\mathcal{U}}_2^d$, there exists a graph $G^* \in \widetilde{\mathcal{U}}_3^d$ such that $\mu_1(G) < \mu_1(G^*)$.*

Proof. For any graph $G \in U_2(p_2, \ldots, p_d, p_{d+2}, p_{d+3}) \subseteq \widetilde{\mathcal{U}}_2^d$, let T_i be the tree attached to the vertex v_i of U_2, for $i = 2, \ldots, d, d+2, d+3$. Let $C = v_k v_{d+2} v_{d+3} v_k$ be the unique cycle of G. Suppose $G' \in U_2(p_2, \ldots, p_{k-1}, p_k + p_{d+2} + p_{d+3}, p_{k+1}, \ldots, p_d, 0, 0)$ and $T'_i \cong T_i$ for $i = 2, \ldots, k-1, k+1, \ldots, d$, where T'_i is the tree attached to the vertex v_i of G', and T'_k is obtained from T_k, T_{d+2}, T_{d+3} by identifying the vertices v_k, v_{d+2} and v_{d+3}. Then by Lemma 3.4, $\mu_1(G) \leqslant \mu_1(G')$. Let $G'' = G' - v_{d+2}v_{d+3}$. Then $N_{G''}(v_{d+2}) = N_{G''}(v_{d+3}) = \{v_k\}$. From G'' to G', by Lemma 2.7, the eigenvalue of G'' that increased by 2 is given by $d(v_{d+2})$. By Lemma 2.8, $\mu_1(G'') > \Delta(G'') + 1 \geqslant 4 \geqslant d_{G''}(v_{d+2}) + 2$, this means that $\mu_1(G') = \mu_1(G'')$. If $k \leqslant d-1$, let $G''' = G'' + v_{k+1}v_{d+3}$; if $k = d$, let $G''' = G'' + v_{k-1}v_{d+2}$. Then, in either case, by Lemma 2.1, $\mu_1(G'') \leqslant \mu_1(G''')$ and $G''' \in \widetilde{\mathcal{U}}_1^d$. By Lemma 3.1, we can get that there exists a graph $G^* \in \widetilde{\mathcal{U}}_3^d$ such that $\mu_1(G''') < \mu_1(G^*)$. So $\mu_1(G) < \mu_1(G^*)$. $\square$

Let $B_n = L_v(P_{n+1})(n \geqslant 1)$, where P_{n+1} is a path with $n+1$ vertices and v is one of the end vertices of P_{n+1}. Then

Lemma 4.3 ([10]). *Set $\Phi(P_0) = 0$, $\Phi(B_0) = 1$. We have*

(1) $\Phi(P_{n+1}) = (x-2)\Phi(P_n) - \Phi(P_{n-1})$;

(2) $x\Phi(B_n) = \Phi(P_{n+1}) + \Phi(P_n)$.

Lemma 4.4 ([10]). *For $m \geqslant 2$, $n \geqslant 1$ and $x \neq 0, 2$, we have*

(1) $\Phi(B_m)\Phi(P_n) - \Phi(B_{m-1})\Phi(P_{n+1}) = \Phi(B_{m-1})\Phi(P_{n-1}) - \Phi(B_{m-2})\Phi(P_n)$;

(2) $\Phi(B_m)\Phi(B_n) - \Phi(B_{m-1})\Phi(B_{n+1}) = \Phi(B_{m-1})\Phi(B_{n-1}) - \Phi(B_{m-2})\Phi(B_n)$.

The above two lemmas will be frequently used in the proofs of the following lemma.

Lemma 4.5. *For any graph $G \in \widetilde{\mathcal{U}}_3^d$, $3 \leqslant d \leqslant n-3$, we have*

$$\mu_1(G) \leqslant \mu_1(\Diamond_n^d),$$

and the equality holds if and only if $G \cong \Diamond_n^d$.

Proof. Let $G \in \widetilde{\mathcal{U}}_3^d$, $3 \leqslant d \leqslant n-3$ and $X = (x_1, x_2, \ldots, x_n)^t$ a unit eigenvector of G corresponding to $\mu_1(G)$, where x_i corresponds to the vertex $v_i (1 \leqslant i \leqslant n)$.

Choose $G \in \widetilde{\mathcal{U}}_3^d$ such that the Laplacian spectral radius of G is as large as possible. Similar to Lemma 4.1, we can assume that each $T_i (2 \leqslant i \leqslant d+2, i \neq d+1)$ is a star, if T_i is not a single vertex. $\square$

Fact 1. $G \in \overline{\mathcal{U}}_3^d$.

Proof. Otherwise, there must exist some $2 \leqslant i, j \leqslant d+2, i, j \neq d+1$ such that $p_i > 0$ and $p_j > 0$. Suppose $V(T_i) \setminus \{v_i\} = \{u_1, \ldots, u_s\}$, $V(T_j) \setminus \{v_j\} = \{w_1, \ldots, w_t\}$. Let X be a unit eigenvector of G corresponding to $\mu_1(G)$.

If $|x_{v_i}| \geqslant |x_{v_j}|$, let $G^* = G - v_j w_1 - \cdots - v_j w_t + v_i w_1 + \cdots + v_i w_t$.

If $|x_{v_i}| < |x_{v_j}|$, let $G^* = G - v_i u_1 - \cdots - v_i u_s + v_j u_1 + \cdots + v_j u_s$.

Then, in either case, G^* is still a bipartite graph and $G^* \in \widetilde{\mathcal{U}}_3^d$, by Lemma 2.12, we have $\mu_1(G) < \mu_1(G^*)$, which is a contradiction. $\square$

So we assume that $G \in \overline{\mathcal{U}}_3^d$ is a graph obtained from U_3 by attaching $n-d-2$ pendent vertices to v_i for some i. Let $P = v_1 v_2 \cdots v_k v_{k+1} \cdots v_d v_{d+1}$ be an induced path of G with $d(v_1) = 1$ and $C = v_k v_{k+1} v_{k+2} v_{d+2} v_k$ the only cycle of G.

Fact 2. If $p_i > 0$, then $i \in \{k, k+2\}$.

Proof. We first show that $i \in \{k, k+2, d+2\}$.

Otherwise, without loss of generality, we may assume that $2 \leqslant i < k$. Then by Corollary 2.11, $\mu_1(G^{v_i v_{i+1}}(w)) > \mu_1(G)$ and the diameter of $G^{v_i v_{i+1}}(w)$ is $d-1$. Let $G^* = G^{v_i v_{i+1}}(w) + v_1 u$, where u is a new vertex different from the vertices of $G^{v_i v_{i+1}}(w)$. Then $G^* \in \overline{\mathcal{U}}_3^d$ and $G^{v_i v_{i+1}}(w)$ is a proper subgraph of G^*. Since G^* is a bipartite graph, by Lemma 2.14, $\mu_1(G^*) > \mu_1(G^{v_i v_{i+1}}(w)) > \mu_1(G)$, a contradiction.

Let $t = n-d-2$ and $l = d-k$. Since $p_i > 0$, we get $t \geqslant 1$. Let $G_i (i = 1, 2, 3)$ be defined as in Fig. 6 and $G'(G'')$ the graph obtained from $G_1(G_2)$ by deleting the vertices $v_1, \ldots, v_{k-1}, v_{k+3}, \ldots, v_{d+1}$.

We first consider G_1 and G_2. If $l = 1$, let X be a unit eigenvector of G_2 corresponding to $\mu_1(G_2)$.

If $|x_{v_k}| \geqslant |x_{v_{d+2}}|$, let $G^{**} = G_2 - v_{d+2}v_{d+3} - \cdots - v_{d+2}v_n + v_k v_{d+3} + \cdots + v_k v_n$.

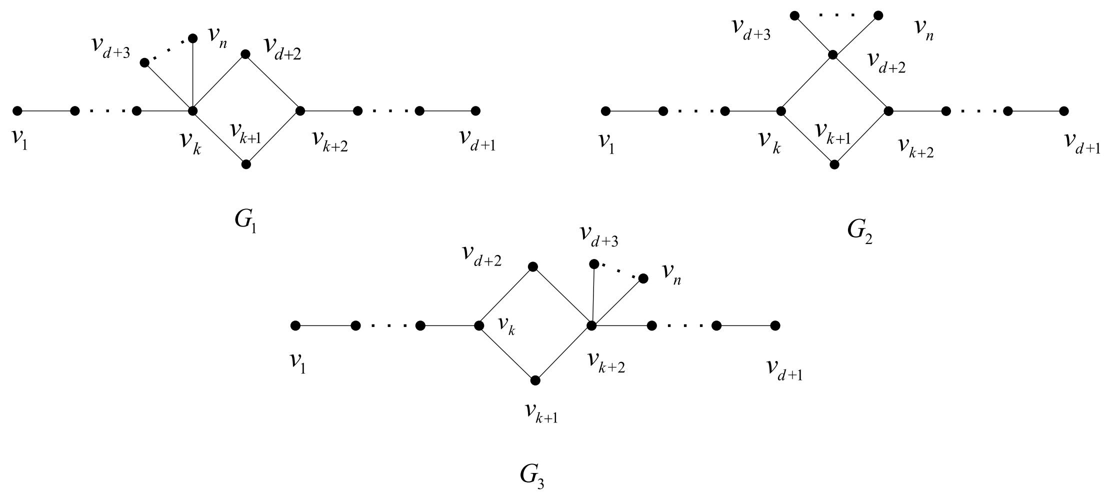

Fig. 6. Graphs G_1, G_2 and G_3.

If $|x_{v_k}| < |x_{v_{d+2}}|$, let $G^{**} = G_2 - v_kv_{k-1} + v_{d+2}v_{k-1}$.
Then, in either case, $G^{**} \cong G_1$ and by Lemma 2.12, we have $\mu_1(G_2) < \mu_1(G^{**})$. So $\mu_1(G_2) < \mu_1(G_1)$.
In the following, we consider that $l \geqslant 2$. By Lemma 3.1, we have

$$\begin{aligned}
\Phi(G_1) &= \Phi(G'v_{k+2} : v_{k+2}P_l)\Phi(B_{k-1}) + \Phi(L_{v_k}(G'v_{k+2} : v_{k+2}P_l))(\Phi(P_k) - x\Phi(B_{k-1})) \\
&= \Phi(B_{k-1})[\Phi(G')\Phi(B_{l-1}) - \Phi(L_{v_{k+2}}(G'))\Phi(P_{l-1})] \\
&\quad - (x-1)^t\Phi(P_{k-1})[\Phi(L_{v_k}(C))\Phi(B_{l-1}) - \Phi(L_{v_k,v_{k+2}}(C))\Phi(P_{l-1})]; \\
\Phi(G_2) &= \Phi(G''v_{k+2} : v_{k+2}P_l)\Phi(B_{k-1}) + \Phi(L_{v_k}(G''v_{k+2} : v_{k+2}P_l))(\Phi(P_k) - x\Phi(B_{k-1})) \\
&= \Phi(B_{k-1})[\Phi(G'')\Phi(B_{l-1}) - \Phi(L_{v_{k+2}}(G''))\Phi(P_{l-1})] \\
&\quad - \Phi(P_{k-1})[\Phi(L_{v_k}(G''))\Phi(B_{l-1}) - \Phi(L_{v_k,v_{k+2}}(G''))\Phi(P_{l-1})].
\end{aligned}$$

Since G' and G'' are two graphs obtained from $C = v_kv_{k+1}v_{k+2}v_{d+2}v_k$ by attaching $n-d-2$ pendent vertices to vertex v_k and v_{d+2}, respectively, G' is the isomorphism to G''. By Lemma 3.1, we have

$$\Phi(G') = \Phi(G'');$$
$$\Phi(L_{v_{k+2}}(G')) = (x-1)^t\Phi(L_{v_{k+2}}(C)) - tx(x-1)^{t-1}\Phi(L_{v_{k+2},v_k}(C));$$
$$\Phi(L_{v_k}(G')) = (x-1)^t\Phi(L_{v_k}(C));$$
$$\Phi(L_{v_{k+2}}(G'')) = \Phi(L_{v_k}(G'')) = (x-1)^t\Phi(L_{v_{k+2}}(C)) - tx(x-1)^{t-1}\Phi(L_{v_{d+2},v_k}(C));$$
$$\Phi(L_{v_k,v_{k+2}}(G'')) = (x-2)(x-1)^{t-1}[(x-2)(x-1) - tx].$$
$$\begin{aligned}
\Phi(G_1) - \Phi(G_2) &= \Phi(B_{k-1})\Phi(P_{l-1})(\Phi(L_{v_{k+2}}(G'')) - \Phi(L_{v_{k+2}}(G'))) + \Phi(P_{k-1})\Phi(B_{l-1})[-(x-1)^t\Phi(L_{v_k}(C)) \\
&\quad + \Phi(L_{v_k}(G''))] + \Phi(P_{k-1})\Phi(P_{l-1})[(x-1)^t\Phi(L_{v_k,v_{k+2}}(C)) - \Phi(L_{v_k,v_{k+2}}(G''))] \\
&= tx(x-1)^{t-1}[\Phi(B_{k-1})\Phi(P_{l-1}) - (x^2-4x+3)\Phi(P_{k-1})\Phi(B_{l-1}) + (x-2)\Phi(P_{k-1})\Phi(P_{l-1})].
\end{aligned}$$

By Lemma 4.3, we can get $\Phi(P_n) = \Phi(B_n) + \Phi(B_{n-1})$ for $n \geqslant 1$. So

$$\begin{aligned}
&\Phi(B_{k-1})\Phi(P_{l-1}) - (x^2-4x+3)\Phi(P_{k-1})\Phi(B_{l-1}) + (x-2)\Phi(P_{k-1})\Phi(P_{l-1}) \\
&\quad = \Phi(B_{k-1})(\Phi(B_{l-1}) + \Phi(B_{l-2})) - (x^2-5x+5)(\Phi(B_{k-1}) + \Phi(B_{k-2}))\Phi(B_{l-1}) \\
&\qquad + (x-2)(\Phi(B_{k-1}) + \Phi(B_{k-2}))(\Phi(B_{l-1}) + \Phi(B_{l-2})) \\
&\quad = (x-1)\Phi(B_{k-1})\Phi(B_{l-2}) + (x-2)\Phi(B_{k-2})\Phi(B_{l-2}) - (x^2-5x+4)\Phi(B_{k-1})\Phi(B_{l-1}) \\
&\qquad - (x^2-5x+5)\Phi(B_{k-2})\Phi(B_{l-1}).
\end{aligned} \tag{4.1}$$

If $l = 2$, since $\Phi(B_0) = 1$ and $\Phi(B_1) = x-1$,

$$\begin{aligned}
(4.1) &= (x-1)\Phi(B_{k-1}) - (x^2-5x+4)(x-1)\Phi(B_{k-1}) + (x-2)\Phi(B_{k-2}) - (x^2-5x+5)(x-1)\Phi(B_{k-2}) \\
&= -(x-1)(x^2-5x+3)\Phi(B_{k-1}) - (x-1)(x^2-5x+4)\Phi(B_{k-2}) - \Phi(B_{k-2}) \\
&< 0,
\end{aligned}$$

for all $x \geqslant \mu_1(G) \geqslant 5$.

If $l > 2$, by Lemma 4.3, $\Phi(B_{l-1}) = (x-2)\Phi(B_{l-2}) - \Phi(B_{l-3})$,

$$\begin{aligned}(4.1) = {} & (x-1)\Phi(B_{k-1})\Phi(B_{l-2}) - (x^2-5x+4)\Phi(B_{k-1})\Phi(B_{l-1}) \\ & + \Phi(B_{k-2})\Phi(B_{l-3}) - (x^2-5x+4)\Phi(B_{k-2})\Phi(B_{l-1}).\end{aligned}$$

Since $\mu_1(P_n) \leqslant 4$, by Lemma 2.3, $\Phi(B_m) \leqslant 4 (m \leqslant n)$ and $\Phi(B_{l-1}) \geqslant \Phi(B_{l-2}) \geqslant \Phi(B_{l-3})$, for all $x \geqslant \mu_1(G) \geqslant 5$. So

$$\begin{aligned}&(x-1)\Phi(B_{k-1})\Phi(B_{l-2}) - (x^2-5x+4)\Phi(B_{k-1})\Phi(B_{l-1}) < 0, \\ &\Phi(B_{k-2})\Phi(B_{l-3}) - (x^2-5x+4)\Phi(B_{k-2})\Phi(B_{l-1}) < 0.\end{aligned}$$

So, in this case Eq. (4.1) < 0 for all $x \geqslant \mu_1(G) \geqslant 5$.

Combining the above arguments, we get $\Phi(G_1) - \Phi(G_2) < 0$, for all $x \geqslant \mu_1(G) \geqslant 5$.

By Lemma 2.2, $\mu_1(G_1) > \mu_1(G_2)$.

In a similar way, we can prove that $\mu_1(G_3) > \mu_1(G_2)$. □

Fact 3. $k = \lceil \frac{d}{2} \rceil$.

Proof. Let G_1 and G' be defined as in above. Let $G_{k,l} := G_1$, where $l = d - k$ and $k \geqslant l \geqslant 2$. Then $G_{k+1,l-1} \cong G_{k,l} - v_d v_{d+1} + v_1 v_{d+1}$. By Lemma 3.1, we have

$$\begin{aligned}\Phi(G_{k,l}) = {} & \Phi(B_{k-1})[\Phi(G')\Phi(B_{l-1}) - \Phi(L_{v_{k+2}}(G'))\Phi(P_{l-1})] \\ & - \Phi(P_{k-1})[\Phi(L_{v_k}(G'))\Phi(B_{l-1}) - \Phi(L_{v_k,v_{k+2}}(G'))\Phi(P_{l-1})];\end{aligned}$$

$$\begin{aligned}\Phi(G_{k+1,l-1}) = {} & \Phi(B_k)[\Phi(G')\Phi(B_{l-2}) - \Phi(L_{v_{k+2}}(G'))\Phi(P_{l-2})] \\ & - \Phi(P_k)[\Phi(L_{v_k}(G'))\Phi(B_{l-2}) - \Phi(L_{v_k,v_{k+2}}(G'))\Phi(P_{l-2})].\end{aligned}$$

$$\Phi(G') = x(x-2)(x-1)^{t-1}[(x-1-t)(x^2-4x+2) - 2(x-3)(x-1)];$$

$$\Phi(L_{v_k}(G')) = (x-1)^t(x-2)(x^2-4x+2);$$

$$\Phi(L_{v_{k+2}}(G')) = (x-1)^{t-1}(x-2)[(x-1)(x^2-4x+2) - tx(x-2)];$$

$$\Phi(L_{v_k,v_{k+2}}(G')) = (x-1)^t(x-2)^2.$$

$$\begin{aligned}\Phi(G_{k,l}) - \Phi(G_{k+1,l-1}) = {} & [\Phi(B_{k-1})\Phi(B_{l-1}) - \Phi(B_k)\Phi(B_{l-2})]\Phi(G') - [\Phi(B_{k-1})\Phi(P_{l-1}) \\ & - \Phi(B_k)\Phi(P_{l-2})]\Phi(L_{v_{k+2}}(G')) - [\Phi(P_{k-1})\Phi(B_{l-1}) - \Phi(P_k)\Phi(B_{l-2})]\Phi(L_{v_k}(G')) \\ & + [\Phi(P_{k-1})\Phi(P_{l-1}) - \Phi(P_k)\Phi(P_{l-2})]\Phi(L_{v_k,v_{k+2}}(G')) \\ = {} & [\Phi(B_{k-l+1})\Phi(B_1) - \Phi(B_{k-l+2})\Phi(B_0)]\Phi(G') + [\Phi(B_{k-l+2})\Phi(P_0) \\ & - \Phi(B_{k-l+1})\Phi(P_1)]\Phi(L_{v_{k+2}}(G')) - [\Phi(P_{k-l+1})\Phi(B_1) - \Phi(P_{k-l+2})\Phi(B_0)]\Phi(L_{v_k}(G')) \\ & - [\Phi(P_{k-l+2})\Phi(P_0) - \Phi(P_{k-l+1})\Phi(P_1)]\Phi(L_{v_k,v_{k+2}}(G')) \\ = {} & [(x-1)\Phi(B_{k-l+1}) - \Phi(B_{k-l+2})]\Phi(G') - x\Phi(B_{k-l+1})\Phi(L_{v_{k+2}}(G')) \\ & - [(x-1)\Phi(P_{k-l+1}) - \Phi(P_{k-l+2})]\Phi(L_{v_k}(G')) + x\Phi(P_{k-l+1})\Phi(L_{v_k,v_{k+2}}(G')) \\ = {} & \Phi(G')\Phi(P_{k-l+1}) - [(x-1)\Phi(P_{k-l+1}) - \Phi(P_{k-l})]\Phi(L_{v_{k+2}}(G')) \\ & - [\Phi(P_{k-l+1}) + \Phi(P_{k-l})]\Phi(L_{v_k}(G')) + x\Phi(P_{k-l+1})\Phi(L_{v_k,v_{k+2}}(G')) \\ = {} & \Phi(P_{k-l+1})[\Phi(G') - (x-1)\Phi(L_{v_{k+2}}(G')) - \Phi(L_{v_k}(G')) + x\Phi(L_{v_k,v_{k+2}}(G'))] \\ & + \Phi(P_{k-l})[\Phi(L_{v_{k+2}}(G')) - \Phi(L_{v_k}(G'))]. \\ = {} & \Phi(P_{k-l+1})[tx(x-1)^{t-1}(x-2) - x(x-1)^t(x-2)(x-4-t)] \\ & - tx(x-1)^{t-1}(x-2)^2\Phi(P_{k-l}) \\ = {} & -x(x-1)^{t-1}(x-2)[t\Phi(P_{k-l-1}) + (x-1)(x-4-t)\Phi(P_{k-l+1})] \\ < {} & 0,\end{aligned}$$

for all $x \geqslant \mu_1(G_{k,l}) > \Delta(G_{k,l}) + 1 = t + 4$.

By Lemma 2.2, $\mu_1(G_{k,l}) > \mu_1(G_{k+1,l-1})$. □

Combining the above arguments, we get the result.

Theorem 4.6. *Let G be a graph in $\mathcal{U}_n^d$, $3 \leqslant d \leqslant n-3$. Then*

$$\mu_1(G) \leqslant \mu_1(\Diamond_n^d),$$

and the equality holds if and only if $G \cong \Diamond_n^d$.

Proof. Since $d_1(\Diamond_n^d) = n - d + 1 \neq n - 1 (d \geqslant 3)$, by Lemma 2.8 (i), we know that $\mu_1(\Diamond_n^d) > n - d + 2$.

Choose $G \in \mathcal{U}_n^d$ such that the Laplacian spectral radius of G is as large as possible. Then by Lemma 2.15, we can assume that $G \neq C_n$.

Let $P_{d+1} = v_1v_2\cdots v_{d+1}$ be the induced path of length d and C_q the unique cycle in G. Since $G \neq C_n$, we have $\min\{d(v_1), d(v_{d+1})\} = 1$, say $d(v_1) = 1$. Suppose u and v are two vertices of G, and $\{d(u), d(v)\} = \{d_1(G), d_2(G)\}$, then

$$d_1(G) + d_2(G) = |N(u)| + |N(v)| = |N(u) \cap N(v)| + |N(u) \cup N(v)|. \tag{4.2}$$

We first prove the following claims.

Claim 1. $|V(C_q) \setminus V(P_{d+1})| \leqslant 2$.

Proof. Otherwise, $|V(C_q) \setminus V(P_{d+1})| \geqslant 3$. There are three cases:

Case 1. Only one vertex of u and v belongs to $V(C_q) \setminus V(P_{d+1})$.

Without loss of generality, we may assume that $u \in V(C_q) \setminus V(P_{d+1})$.

If u is adjacent to v, then $|N(u) \cap N(v)| = 0$, and

$$N(u) \cup N(v) \subseteq (V(G) \setminus V(P_{d+1})) \cup \{v\} \cup N_{P_{d+1}}(v).$$

Combining this equation with Eq. (4.2), we get

$$d_1(G) + d_2(G) \leqslant n - d + 2.$$

By Lemma 2.8(ii), we get

$$\mu_1(G) \leqslant d_1(G) + d_2(G) \leqslant n - d + 2 < \mu_1(\Diamond_n^d),$$

which is a contradiction.

If u is nonadjacent to v, then $|N(u) \cap N(v)| \leqslant 2$, and

$$N(u) \cup N(v) \subseteq (V(G) \setminus (V(P_{d+1}) \cup \{u\})) \cup N_{P_{d+1}}(v).$$

Similar to the above, we can get a contradiction.

Case 2. Neither u nor v belong to $V(C_q) \setminus V(P_{d+1})$.

Then $|N(u) \cap N(v)| \leqslant 1$, and

$$N(u) \cup N(v) \subseteq \big(V(G) \setminus (V(P_{d+1}) \cup V(C_q))\big) \cup N_{P_{d+1} \cup C_q}(v) \cup N_{P_{d+1} \cup C_q}(u).$$

Since $|N_{P_{d+1} \cup C_q}(u)| \leqslant 2$ and $|N_{P_{d+1} \cup C_q}(v)| \leqslant 2$, similar to the above, we can get a contradiction.

Case 3. Both u and v belong to $V(C_q) \setminus V(P_{d+1})$.

Then $|N(u) \cap N(v)| \leqslant 1$, and

$$N(u) \cup N(v) \subseteq V(G) \setminus V(P_{d+1}) \cup N_{P_{d+1}}(u) \cup N_{P_{d+1}}(v).$$

Since $|N_{P_{d+1}} \cup C_q(u)| \leqslant 1$ and $|N_{P_{d+1}} \cup C_q(v)| \leqslant 1$, similar to the above, we can get a contradiction.

Up until now, we have proved Claim 1. □

Claim 2. $|V(C_q) \setminus V(P_{d+1})| \neq 2$.

Proof. Otherwise, $|V(C_q) \setminus V(P_{d+1})| = 2$. Then $|V(C_q) \cap V(P_{d+1})| = 1$ or $|V(C_q) \cap V(P_{d+1})| = 2$.

Case 1. $|V(C_q) \cap V(P_{d+1})| = 1$.

Then $G \in \widetilde{\mathcal{U}}_2^d$. By Lemma 4.2, there exists a graph $G^* \in \widetilde{\mathcal{U}}_3^d$ such that $\mu_1(G) < \mu_1(G^*)$, which is a contradiction.

Case 2. $|V(C_q) \cap V(P_{d+1})| = 2$.

Then $|V(C_q)| = 4$. So in this case, G is a bipartite graph.

If $d = 3$, then $G \in \widetilde{\mathcal{U}}_3^3$. By Lemma 4.5, we have $\mu_1(G) < \mu_1(\Diamond_n^3)$, which is a contradiction.

If $d \geqslant 4$, let $C_q = v_kv_{k+1}u_1u_2v_k$, where $\{v_k, v_{k+1}\} \in V(P_{d+1})$ and $\{u_1, u_2\} = V(C_q) \cap V(P_{d+1})$. Since $d \geqslant 4$, we may assume that $1 \leqslant k \leqslant d - 2$. Let X be a unit eigenvector of G corresponding to $\mu_1(G)$. If $|x_{v_{k+2}}| \leqslant |x_{u_1}|$, let

$$G' = G - v_{k+2}v_{k+3} + u_1v_{k+3};$$

if $|x_{v_{k+2}}| > |x_{u_1}|$, let

$$G' = G - u_1u_2 + v_{k+2}u_2.$$

Then, in either case, $G' \in \mathcal{U}_n^d$ and G' is still a bipartite graph, by Lemma 2.12, we have $\mu_1(G) < \mu_1(G')$, which is a contradiction.

Up until now, we have proved Claim 2. □

Combining Claims 1 and 2, we get $|V(C_q) \setminus V(P_{d+1})| = 1$. So $G \in \widetilde{\mathcal{U}}_1^d$ or $G \in \widetilde{\mathcal{U}}_3^d$. By Lemmas 4.1 and 4.5, we get

$$\mu_1(G) \leqslant \mu_1(\Diamond_n^d),$$

and the equality holds if and only if $G \cong \Diamond_n^d$.

This completes the proof. □

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